

AMENDMENTS TO THE CLAIMS

This listing of claims replaces all prior versions and listings of claims in the application:

1. (Currently amended) A computer-implemented method for generating a library design for a combinatorial library of materials, comprising:

providing a graphical user interface including a workspace for designing a library of materials;

defining one or more sources and one or more destinations, each source being electronic data representing a ~~component~~ chemical or mixture of chemicals to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

displaying a visual representation of one or more of the defined destinations in the workspace of the graphical user interface, each destination representation including a representation of one or more cells in the corresponding arrangement;

receiving user input defining a first mapping, the first mapping being electronic data defining a gradient distribution pattern for assigning a ~~component~~ first chemical or mixture of chemicals represented by one of the defined sources to a plurality of cells in ~~the arrangements represented by the defined destinations~~, the input specifying ~~a set of the gradient distribution pattern according to parameters defining~~ a minimum and a maximum amount of the ~~component~~ first chemical or mixture of chemicals to be assigned to any of the plurality of cells in the corresponding destination ~~of the arrangements~~ and a gradient to be applied between the minimum and maximum amounts of the ~~component~~ first chemical or mixture of chemicals across the plurality of cells;

using the first mapping to calculate amounts of the first chemical or mixture of chemicals to be deposited in each of the plurality of cells; and

~~generating a representation of the library design, the representation comprising electronic data representing the sources, the destinations and the first mapping~~

modifying the visual representation of the defined destinations to include a visual indication of the calculated amounts.

Claim 2. Cancelled.

3. (Currently amended) The method of claim 1, wherein the ~~representation defining the sources and destinations~~ comprises ~~electronic data representing receiving user input specifying one or more sets of properties, each set of properties being associated with one of the sources, the and destinations or the mapping.~~ receiving user input specifying one or more sets of properties, each set of properties being associated with one of the sources, the and destinations or the mapping.

4. (Original) The method of claim 1, wherein defining the sources and destinations comprises receiving an input from a graphical input device.

5. (Currently amended) The method of claim 1, wherein the input defining a first mapping comprises a selection from a set of available mapping types, the set of available mapping types comprising a one to one mapping of a ~~component~~ chemical or mixture of chemicals from a source to a cell in the arrangements and a one to many mapping of a ~~component~~ chemical or mixture of chemicals from a source to a plurality of cells in the arrangements.

6. (Currently amended) The method of claim 5, wherein the set of available mapping types further comprises a many to many mapping of a plurality of ~~components~~ chemicals or mixtures of chemicals from a plurality of sources to a plurality of cells in the arrangements.

7. (Currently amended) The method of claim 6, wherein the set of available mapping types further comprises a many to one mapping of a plurality of ~~components~~ chemicals or mixtures of chemicals from a plurality of sources to a cell in the arrangements.

8. (Original) The method of claim 5, wherein the set of available mapping types further comprises a set of one or more user-defined equations.

9. (Original) The method of claim 1, wherein the gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

Claim 10. Cancelled.

11. (Currently amended) The method of claim 1, further comprising:

receiving second user input defining a second mapping, the second mapping being electronic data defining a second distribution pattern ~~for distributing~~ describing an amount or amounts of a second ~~component~~ chemical or mixture of chemicals to be distributed to one or more cells in the arrangements;

~~wherein generating a representation of the library design includes generating a representation comprising electronic data representing the sources, the destinations and the first and second mappings~~ modifying the visual representation of the defined destinations includes modifying the visual representation to include a visual indication of the amounts of the first and second chemicals or mixtures of chemicals.

12. (Currently amended) The method of claim 11, wherein the second distribution pattern ~~for assigning a second component~~ includes electronic data identifying a fixed amount of the second ~~component~~ chemical or mixture of chemicals to be assigned distributed to one or more cells in the arrangements.

13. (Currently amended) The method of claim 11, wherein the second input specifies a second gradient distribution pattern according to set of gradient parameters defining a minimum and a maximum amount of the second ~~component~~ chemical or mixture of chemicals to be assigned to a second plurality of cells of the arrangements and a second gradient to be applied between the minimum and maximum amounts of the second ~~component~~ chemical or mixture of chemicals across the second plurality of cells.

14. (Currently amended) The method of claim ~~1~~ 91, further comprising ~~generating a modified library design by:~~

receiving user input ~~redefining a source, a destination or a mapping~~ modifying

one or more of the plurality of mappings; and

generating a representation of the modified library design modifying the visual representation of the defined destinations according to the modified mappings.

Claims 15-18. Cancelled.

19. (Currently Amended) A computer-implemented method for generating a library design for a combinatorial library of materials, comprising:

providing a graphical user interface including a workspace for designing a library of materials;

defining a set of one or more sources and one or more destinations, each source being electronic data representing a component chemical or mixture of chemicals to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

displaying a visual representation of one or more of the defined destinations in the workspace of the graphical user interface, each destination representation including a representation of one or more destination areas, each destination area including one or more cells in the corresponding arrangement;

receiving user input defining a set of first mappings, the input specifying a set plurality of equations and associating one or more of the plurality of equations with one or more of the destination areas;

solving the plurality of equations to calculate amounts for calculating an amount of one or more first chemicals or mixtures of chemicals components represented by the defined sources to be assigned to one or more cells in the arrangements represented by the defined destinations, the amounts of the one or more first chemicals or mixtures of chemicals to be assigned to a given cell in the arrangements being calculated according to the equations associated with the area or areas including the cell; and

generating a representation of the library design, the representation comprising electronic data representing the sources, the destinations and the first mappings

modifying the visual representation of the defined destinations to include a visual indication of the calculated amounts.

20. Cancelled.

21. (Currently amended) The method of claim 19, wherein the first chemical or mixture of chemicals ~~component~~ to be assigned to a cell in the arrangement is determined by the location of the cell within the corresponding arrangement.

22. (Currently amended) The method of claim 21, wherein the composition of a material is determined using a subset of the set plurality of equations, the subset of equations being determined by the location of the cell within the corresponding arrangement.

23. (Currently amended) The method of claim 19, further comprising:
generating an error indicator signal if the ~~number of equations in the set plurality~~ of equations is ~~not equal to the number of sources in the set of sources~~ cannot be solved for each cell in the arrangements.

24. (Currently amended) The method of claim 19, wherein at least one of the set plurality of equations is selected from the group consisting of:

a ratio equation defining an amount of ~~a component~~ one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of an amount of another ~~component~~ chemical or mixture of chemicals to be assigned to the cell;

a volume equation defining an amount of ~~a component~~ one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total volume of a plurality of ~~components~~ chemicals or mixtures of chemicals to be assigned to the cell;
and

a mass equation defining an amount of ~~a component~~ one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total mass of a plurality of ~~components~~ chemicals or mixtures of chemicals to be assigned to the cell.

Claims 25-26. Cancelled.

27. (Currently amended) The method of claim 19, wherein ~~using the set of equations to calculate a composition of a material assigned to one or more of the cells~~ solving the plurality of equations comprises ~~simultaneously solving a set of interdependent~~ using matrix algebra techniques to solve the plurality of equations.

Claim 28. Cancelled.

29. (Currently amended) The method of claim 19, further comprising:
receiving an input defining a ~~second~~ gradient mapping, the ~~second~~ gradient mapping being electronic data defining a distribution pattern for distributing a second chemical or mixture of chemicals component to cells in the arrangements, the distribution pattern including a minimum and a maximum amount of the second chemical or mixture of chemicals component to be assigned to any of a plurality of cells of the arrangements and a gradient to be applied between the minimum and maximum amounts of the second chemical or mixture of chemicals component across the plurality of cells; and
using the second mapping to calculate amounts of the second chemical or mixture of chemicals to be deposited in each of the plurality of cells;
wherein ~~generating a representation of the library design includes generating a representation comprising electronic data representing the sources, the destinations, the first set of mappings and the second mapping~~ modifying the visual representation of the defined destinations comprises modifying the visual representation to include a visual indication of the calculated amounts of the first and second chemicals or mixtures of chemicals.

Claims 30-36. Cancelled.

37. (Currently amended) A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

provide a graphical user interface including a workspace for designing a library of materials;

receive an input defining one or more sources and one or more destinations, each source being electronic data representing a ~~component~~ chemical or mixture of chemicals to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

display a visual representation of one or more of the defined destinations in the workspace of the graphical user interface, each destination representation including a representation of one or more cells in the corresponding arrangement;

receive user input defining a first mapping, the first mapping being electronic data defining a gradient distribution pattern for assigning a ~~component~~ first chemical or mixture of chemicals represented by one of the defined sources to a plurality of cells in ~~the arrangements represented by the defined destinations~~, the input specifying a ~~set of the gradient distribution pattern according to parameters defining~~ a minimum and a maximum amount of the ~~component~~ first chemical or mixture of chemicals to be assigned to any of the plurality of cells in the corresponding destination ~~of the arrangements~~ and a gradient to be applied between the minimum and maximum amounts of the ~~component~~ first chemical or mixture of chemicals across the plurality of cells;

use the first mapping to calculate amounts of the first chemical or mixture of chemicals to be deposited in each of the plurality of cells; and

~~generate a representation of the library design, the representation comprising electronic data representing the sources, the destinations and the mapping~~

modify the visual representation of the defined destinations to include a visual indication of the calculated amounts.

38. Cancelled.

39. (Currently amended) The computer program product of claim 37, wherein the ~~representation comprises electronic data representing one or more sets of properties, each set of~~ instructions operable to cause a programmable processor to define the sources and destinations comprise instructions operable to cause a programmable processor to receive

user input specifying properties being associated with one of the sources, the and destinations or the mapping.

40. (Previously presented) The computer program product of claim 37, wherein the input defining the sources and destinations comprises an input from a graphical input device.

41. (Currently amended) The computer program product of claim 37, wherein the input defining a first mapping comprises a selection from a set of available mapping types, the set of available mapping types comprising a one to one mapping of a ~~component~~ chemical or mixture of chemicals from a source to a cell in the arrangements and a one to many mapping of a ~~component~~ chemical or mixture of chemicals from a source to a plurality of cells in the arrangements.

42. (Currently amended) The computer program product of claim 41, wherein the set of available mapping types further comprises a many to many mapping of a plurality of ~~components~~ chemicals or mixtures of chemicals from a plurality of sources to a plurality of cells in the arrangements.

43. (Currently amended) The computer program product of claim 42, wherein the set of available mapping types further comprises a many to one mapping of a plurality of ~~components~~ chemicals or mixtures of chemicals from a plurality of sources to a cell in the arrangements.

44. (Previously presented) The computer program product of claim 40, wherein the set of available mapping types further comprises a set of one or more user-defined equations.

45. (Previously presented) The computer program product of claim 37, wherein the gradient is selected from the group consisting of linear, logarithmic, exponential, polynomial and geometric progression.

46. Cancelled.

47. (Currently amended) The computer program product of claim 37, further comprising instructions operable to cause a programmable processor to:

receive second user input defining a second mapping, the second mapping being electronic data defining a second distribution pattern ~~for distributing~~ describing an amount or amounts of a second ~~component~~ chemical or mixture of chemicals to be distributed to one or more cells in the arrangements;

wherein the instructions operable to cause a programmable processor to ~~generate a representation of the library design~~ modify the visual representation of the defined destinations include instructions operable to cause a programmable processor to ~~generate a representation comprising electronic data representing the sources, the destinations and the first and second mappings~~ modify the visual representation to include a visual indication of the amounts of the first and second chemicals or mixtures of chemicals.

48. (Currently amended) The computer program product of claim 47, wherein the second distribution pattern ~~for assigning a second component~~ includes electronic data identifying a fixed amount of the second ~~component~~ chemical or mixture of chemicals to be ~~assigned~~ distributed to one or more cells in the arrangements.

49. (Currently amended) The computer program product of claim 48, wherein the second input specifies a second gradient distribution pattern according to set of gradient parameters defining a minimum and a maximum amount of the second ~~component~~ chemical or mixture of chemicals to be assigned to a second plurality of cells of the arrangements and a second gradient to be applied between the minimum and maximum amounts of the second ~~component~~ chemical or mixture of chemicals across the second plurality of cells.

50. (Currently amended) The computer program product of claim 96, further comprising instructions operable to cause a programmable processor to:

~~generate a modified library design by receiving~~ receive an input ~~redefining a~~

~~source, a destination or a mapping~~ modifying one or more of the plurality of mappings;
and

~~generating a representation defining the modified library design~~ modify the visual representation of the defined destinations according to the modified mappings.

Claims 51-54. Cancelled.

55. (Currently amended) A computer program product on a computer-readable medium for generating a library design for a combinatorial library of materials, the computer program product comprising instructions operable to cause a programmable processor to:

provide a graphical user interface including a workspace for designing a library of materials;

~~receive user input defining~~ define a set of one or more sources and one or more destinations, each source being electronic data representing a ~~component~~ chemical or mixture of chemicals to be used in preparing the combinatorial library and each destination being electronic data representing an arrangement of cells;

display a visual representation of one or more of the defined destinations in the workspace of the graphical user interface, each destination representation including a representation of one or more destination areas, each destination area including one or more cells in the corresponding arrangement;

~~receive user input defining a set of first mappings, the input specifying a set~~ plurality of equations and associating one or more of the plurality of equations with one or more of the destination areas;

solve the plurality of equations to calculate amounts for calculating an amount of one or more first chemicals or mixtures of chemicals components represented by the defined sources to be assigned to one or more cells in the arrangements represented by the defined destinations, the amounts of the one or more first chemicals or mixtures of chemicals to be assigned to a given cell in the arrangements being calculated according to the equations associated with the area or areas including the cell; and

~~generate a representation of the library design, the representation comprising electronic data representing the sources, the destinations and the first mappings~~
modify the visual representation of the defined destinations to include a visual indication of the calculated amounts.

56. Cancelled.

57. (Currently amended) The computer program product of claim 55, wherein the first chemical or mixture of chemicals ~~component~~ to be assigned to a cell in the arrangement is determined by the location of the cell within the corresponding arrangement.

58. (Currently amended) The computer program product of claim 57, wherein the composition of a material is determined using a subset of the ~~set~~ plurality of equations, the subset of equations being determined by the location of the cell within the corresponding arrangement.

59. (Currently amended) The computer program product of claim 55, further comprising instructions operable to:
generate an error indicator signal if the ~~number of equations in the set~~ plurality of equations is ~~not equal to the number of sources in the set of sources~~ cannot be solved for each cell in the arrangements.

60. (Currently amended) The computer program product of claim 55, wherein at least one of the ~~set~~ plurality of equations is selected from the group consisting of:
a ratio equation defining an amount of a ~~component~~ one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of an amount of another ~~component~~ chemical or mixture of chemicals to be assigned to the cell;
a volume equation defining an amount of a ~~component~~ one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total volume of a plurality of ~~components~~ chemicals or mixtures of chemicals to be assigned to the cell;

and

a mass equation defining an amount of ~~a component~~ one of the first chemicals or mixtures of chemicals to be assigned to a cell as a function of a total mass of a plurality of ~~components~~ chemicals or mixtures of chemicals to be assigned to the cell.

Claims 61-62. Cancelled.

63. (Currently amended) The computer program product of claim 55, wherein the instructions operable to cause a programmable processor to ~~use the set of equations to calculate a composition of a material assigned to one or more of the cells~~ solve the plurality of equations comprise instructions ~~simultaneously to use matrix algebra techniques~~ to solve a set of interdependent the plurality of equations.

Claim 64. Cancelled.

65. (Currently amended) The computer program product of claim 55, further comprising instructions operable to:

receive an input defining a ~~second gradient~~ mapping, the ~~second gradient~~ mapping being electronic data defining a distribution pattern for distributing a second chemical or mixture of chemicals ~~component~~ to cells in the arrangements, the distribution pattern including a minimum and a maximum amount of the second chemical or mixture of chemicals ~~component~~ to be assigned to any of a plurality of cells of the arrangement and a gradient to be applied between the minimum and maximum amounts of the second chemical or mixture of chemicals ~~component~~ across the plurality of cells; and
use the second mapping to calculate amounts of the second chemical or mixture of chemicals to be deposited in each of the plurality of cells;

wherein the instructions operable to cause a programmable processor to ~~generate a representation of the library design~~ modify the visual representation of the defined destinations include instructions operable to cause a programmable processor to ~~generate a representation comprising electronic data representing the sources, the destinations, the first set of mappings and the second mapping~~ modify the visual representation to include

a visual indication of the calculated amounts of the first and second chemicals or mixtures of chemicals.

Claims 66-90. Cancelled.

91. (New) The method of claim 1, wherein:

receiving user input defining a first mapping comprises receiving user input defining a plurality of mappings for assigning to the defined destinations a plurality of chemicals or mixtures of chemicals represented by the defined sources, each of the plurality of mappings including electronic data defining a distribution pattern describing an amount or amounts of one or more of the plurality of chemicals or mixtures of chemicals to a corresponding plurality of cells in the defined destinations; and

modifying the visual representation of the defined destinations includes modifying the visual representation to include a visual indication of the amounts of the plurality of chemicals or mixtures of chemicals.

92. (New) The method of claim 19, further comprising:

receiving user input dividing the destination representations to define the destination areas.

93. (New) The method of claim 19, further comprising:

displaying a visual representation of the defined sources in the workspace of the graphical user interface; and

receiving input associating one or more of the source representations with one or more of the destination areas;

wherein the first chemicals or mixtures of chemicals to be assigned to a given cell in the arrangements are determined by the sources associated with the area or areas that the cell.

94. (New) The method of claim 19, further comprising:

in response to the user input specifying and associating the equations, modifying

the visual representation of the defined destinations to include a visual indication of the equations associated with the destination areas.

95. (New) The method of claim 19, wherein:

defining the sources comprises associating one or more of the chemicals or mixtures of chemicals with a type representing a class of chemicals to be used in preparing the combinatorial library;

receiving user input specifying a plurality of equations comprises receiving user input specifying one or more of the plurality of equations as a function of the type; and

solving the equations comprises solving the equations specified as a function of the type for a given destination area by substituting the corresponding associated chemical or chemicals associated for the type.

96. (New) The computer program product of claim 37, wherein:

the instructions operable to cause a programmable processor to receive user input defining a first mapping comprise instructions operable to cause a programmable processor to receive user input defining a plurality of mappings for assigning to the defined destinations a plurality of chemicals or mixtures of chemicals represented by the defined sources, each of the plurality of mappings including electronic data defining a distribution pattern describing an amount or amounts of one or more of the plurality of chemicals or mixtures of chemicals to a corresponding plurality of cells in the defined destinations; and

the instructions operable to cause a programmable processor to modify the visual representation of the defined destinations comprise instructions operable to cause a programmable processor to modify the visual representation to include a visual indication of the amounts of the plurality of chemicals or mixtures of chemicals.

97. (New) The computer program product of claim 55, further comprising instructions operable to cause a programmable processor to:

receive user input dividing the destination representations to define the destination areas.

98. (New) The computer program product of claim 55, further comprising instructions operable to cause a programmable processor to:

display a visual representation of the defined sources in the workspace of the graphical user interface; and

receive input associating one or more of the source representations with one or more of the destination areas;

wherein the first chemicals or mixtures of chemicals to be assigned to a given cell in the arrangements are determined by the sources associated with the area or areas that the cell.

99. (New) The computer program product of claim 55, further comprising instructions operable to cause a programmable processor to:

modify the visual representation of the defined destinations in response to the user input specifying and associating the equations to include a visual indication of the equations associated with the destination areas.

100. (New) The computer program product of claim 55, wherein:

the instructions operable to cause a programmable processor to define the sources comprise instructions operable to cause a programmable processor to associate one or more of the chemicals or mixtures of chemicals with a type representing a class of chemicals to be used in preparing the combinatorial library;

the instructions operable to cause a programmable processor to receive user input specifying a plurality of equations comprise instructions operable to cause a programmable processor to receive user input specifying one or more of the plurality of equations as a function of the type; and

instructions operable to cause a programmable processor to solve the equations comprise instructions operable to cause a programmable processor to solving the equations specified as a function of the type for a given destination area by substituting the corresponding associated chemical or chemicals associated for the type.